# Explicit solution for a Gaussian wave packet impinging on a square barrier

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**Abstract.** The collision of a quantum Gaussian wave packet with a square barrier is solved explicitly in terms of known functions. The obtained formula is suitable for performing fast calculations or asymptotic analysis. It also provides physical insight since the description of different regimes and collision phenomena typically requires only some of the terms.

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## 1. Introduction

A paradigmatic textbook example [1] of a quantum scattering process is the collision of a particle of mass $m$, initially represented by a minimum-uncertainty-product Gaussian wave packet, with a "square barrier" potential,

$$V(x) = \begin{cases} V_0 & \text{if} \quad -d/2 \leq x \leq d/2 \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

In spite of its simplicity, this model allows to observe and study a number of interesting quantum phenomena, such as tunneling [2, 3, 4, 5, 6, 7, 8, 9], resonances [10], incidence-reflection and incidence-transmission interferences [11], the Hartman effect [12, 4, 13, 14, 15, 16], and time delays or reflection due to a well when the height of the potencial, $V_0$, is negative [17]. It is also used as a standard model to check the validity of approximate numerical methods [18, 19], or to exemplify and test different theories for temporal quantities such as arrival, dwell, or decay times, the asymptotic behaviour at long times [20, 21, 22], and quantum transition state theories [23].

Except for approximate analytical treatments [12], the solution of this time-dependent scattering model has been always obtained by numerical methods, typically using "Fast Fourier Transforms", tridiagonal systems, or by linear combination of the solutions of the stationary Schrödinger equation. Goldberg, Schey, and Schwartz were the first to solve the model by means of a difference equation [17]. While for many purposes these methods may be sufficient, for other applications the numerical approach may be cumbersome, time consuming or even useless. Therefore, an analytical solution in terms of known functions is of much practical interest. In general an analytical solution is not only useful as a fast computational tool; it is also valuable because of the physical insight than can be gained from it, very often by means of approximations that extract the dominant contributions in different limits, parameter ranges and regimes.

In this paper we present an explicit expression in the momentum representation of the time dependence of a Gaussian packet incident on a square barrier in terms of known functions. There are a few other time dependent solvable scattering models: a Lorentzian state impinging on a delta function potential [24, 25, 26] or on a separable exponential potential [26, 27]; and a cutoff plane wave impinging on a square barrier [28, 29], or on a step barrier [30]. While all have been useful and illustrative of several scattering properties, the present model is the only one that combines simultaneously a local potential, resonances, and a physical Hilbert-space initial state with finite moments.

## 2. Explicit solution

The initial wave function is assumed to be a minimum-uncertainty-product Gaussian wave packet located in the left half-line and with negligible overlap with the potential.

In momentum representation it is given by

$$\langle p'|\psi(t=0)\rangle = \left(\frac{2\delta_x}{\pi\hbar^2}\right)^{1/4} \exp\left[-\delta_x\left(p'-p_c\right)^2/\hbar^2 - ip'x_c/\hbar\right], \tag{2}$$

where $x_c$ and $p_c$ are the initial mean position and momentum respectively, and $\delta_x$ is the variance of the state in coordinate representation. Its time evolution can then be written in terms of eigenstates of $H$, $|\phi_{p'}\rangle$ [31, 32], as

$$\psi(p,t) = \int_{-\infty}^{+\infty} \langle p|\phi_{p'}\rangle e^{-iE't/\hbar}\langle p'|\psi(t=0)\rangle\, dp', \tag{3}$$

with $E' \equiv p'^2/2m$. These states are given explicitly in coordinate representation by

$$\langle x|\phi_{p'}\rangle = \frac{1}{h^{1/2}}\begin{cases} Ie^{ip'x/\hbar} + Re^{-ip'x/\hbar} & x < -d/2 \\ Ce^{ip''x/\hbar} + De^{-ip''x/\hbar} & -d/2 \le x \le d/2 \\ Te^{ip'x/\hbar} & x > d/2, \end{cases} \tag{4}$$

where $p'' \equiv \sqrt{p'^2 - 2mV_0}$. The value of the coefficient $I$ will be taken as 1. Note that these (delta-normalized) eigenstates are associated with an incident plane wave of momentum $p'$ for $p' > 0$ and with an outgoing plane wave with momentum $p'$ for $p' < 0$. The coefficients $R$, $C$, $D$ and $T$ are determined by continuity of the wave function and its first derivative,

$$\begin{aligned} R\left(p'\right) &= \frac{i\left(\frac{p''}{p'} - \frac{p'}{p''}\right)\sin\left(p''d/\hbar\right)e^{-ip'd/\hbar}}{2\Omega\left(p'\right)} \\ C\left(p'\right) &= \frac{\left(1+\frac{p'}{p''}\right)e^{-i(p'+p'')d/2\hbar}}{2\Omega\left(p'\right)} \\ D\left(p'\right) &= \frac{\left(1-\frac{p'}{p''}\right)e^{-i(p'-p'')d/2\hbar}}{2\Omega\left(p'\right)} \\ T\left(p'\right) &= \frac{e^{-ip'd/\hbar}}{\Omega\left(p'\right)}, \end{aligned} \tag{5}$$

where

$$\Omega\left(p'\right) \equiv \cos(p''d/\hbar) - \frac{i}{2}\left(\frac{p''}{p'} + \frac{p'}{p''}\right)\sin(p''d/\hbar). \tag{6}$$

Fourier transformation of $\langle x|\phi_{p'}\rangle$ in (4) gives five terms proportional to the coefficients $I, R, T, C, D$ respectively (generically denoted by $A$ hereafter). Substituting these terms into (3) with the initial state in (2), we obtain

$$\psi(p,t) = i\tau\hbar h^{-1/2}\int_{-\infty}^{\infty}\left[g_I\left(p'\right) + g_R\left(p'\right) + g_C\left(p'\right) + g_D\left(p'\right) + g_T\left(p'\right)\right]e^{\phi(p')}dp', \tag{7}$$

where $\tau \equiv (2\pi\hbar)^{-1/2}\left(\frac{2\delta_x}{\pi\hbar^2}\right)^{1/4}$. The term in the exponential $\phi(p')$ is given by

$$\phi\left(p'\right) = \frac{-ip'^2t}{2m\hbar} - \frac{\delta_x\left(p'-p_c\right)^2}{\hbar^2} - \frac{ip'x_c}{\hbar} - \frac{ip'd}{2\hbar}; \tag{8}$$

and

$$
\begin{aligned}
g_I(p') &\equiv \frac{e^{ipd/2\hbar}}{p - p' + i\hbar 0^+} \\
g_R(p') &\equiv \frac{R(p') e^{ip'd/\hbar}\, e^{ipd/2\hbar}}{p + p' + i\hbar 0^+} \\
g_C(p') &\equiv \frac{-2iC(p') e^{ip'd/2\hbar}}{p - p''} \sin[(p - p'')d/2\hbar] \\
g_D(p') &\equiv \frac{-2iD(p') e^{ip'd/2\hbar}}{p + p''} \sin[(p + p'')d/2\hbar] \\
g_T(p') &\equiv \frac{-T(p') e^{ip'd/\hbar}\, e^{-ipd/2\hbar}}{p - p' - i\hbar 0^+}.
\end{aligned} \tag{9}
$$

Note the three explicit ("structural" [33]) poles at $p'_I \equiv p + i\hbar 0^+$, $p'_T \equiv p - i\hbar 0^+$, and $p'_R \equiv -p - i\hbar 0^+$, in addition to the poles of the functions $C$, $D$, $R$ and $T$, $p'_j$ $(j = 1, ..., \infty)$, which are zeros of $\Omega(p')$. All the poles lie in the lower half complex plane except for the incidence pole, $p'_I$.

The integral in Eq. (7) can be solved by completing the square in Eq.(8) and introducing the variable $u$ as

$$
u \equiv \frac{p' - z}{f}, \tag{10}
$$

with

$$
f \equiv \left(\frac{\delta_x}{\hbar^2} + i\frac{t}{2m\hbar}\right)^{-1/2}. \tag{11}
$$

$u$ is zero at the saddle point $z$, defined by

$$
z \equiv \frac{m\left[4mp_c\delta_x^2 - (x_c + d/2)\,\hbar^2 t\right] - i2m\hbar\left[m\delta_x\,(x_c + d/2) + p_c\delta_x t\right]}{4m^2\delta_x^2 + t^2\hbar^2}, \tag{12}
$$

and becomes real along the steepest descent path, a straight line with slope $-t\hbar/(2m\delta_x)$. We now deform the contour and integrate along the steepest descent path, namely along the real $u$ axis,

$$
\begin{aligned}
\psi(p,t) = {} & if\tau\hbar h^{-1/2}\, e^{-\left(\delta_x p_c^2/\hbar^2\right) + \eta^2} \\
& \times \int_{\Gamma_u} \left[g_I(u) + g_R(u) + g_C(u) + g_D(u) + g_T(u)\right] e^{-u^2}\, du,
\end{aligned} \tag{13}
$$

where

$$
\eta \equiv \left(\frac{2p_c\delta_x}{\hbar^2} - i\frac{(x_c + d/2)}{\hbar}\right)\left[4\left(\frac{\delta_x}{\hbar^2} + i\frac{t}{2m\hbar}\right)\right]^{-1/2}, \tag{14}
$$

$g_A(u) \equiv g_A(p' = fu + z)$, and $\Gamma_u$ goes from $-\infty$ to $+\infty$ including a circle around the poles that have been crossed by the contour deformation. Since the $g_I$, $g_R$, $g_T$ and $g_{CD} \equiv g_C + g_D$ are meromorphic functions with simple poles, it is useful to extract explicitly the singularities and leave the remainder as an entire function, $h$,

$$
g_I(u) = \frac{\mathcal{R}_I}{u - u_I}
$$

$$
\begin{aligned}
g_R(u) &= \frac{\mathcal{R}_R}{u-u_R} + \sum_{j=1}^{\infty} \frac{\mathcal{R}_{Rj}}{u-u_j} + h_R(u) \\
g_{CD}(u) &= \sum_{j=1}^{\infty} \frac{\mathcal{R}_{Cj}+\mathcal{R}_{Dj}}{u-u_j} + h_{CD}(u) \\
g_T(u) &= \frac{\mathcal{R}_T}{u-u_T} + \sum_{j=1}^{\infty} \frac{\mathcal{R}_{Tj}}{u-u_j} + h_T(u).
\end{aligned}
\tag{15}
$$

Again the poles in the $u$ complex plane may be separated into "structural" [33],

$$
\begin{aligned}
u_I &= f^{-1}(p+i0^+ - z) \\
u_R &= f^{-1}(-p-i0^+ - z) \\
u_T &= f^{-1}(p-i0^+ - z),
\end{aligned}
\tag{16}
$$

and "resonance" poles (see the Appendix),

$$
u_j = f^{-1}(p'_j - z) \qquad\qquad j = 1, ..., \infty. \tag{17}
$$

The residues $\mathcal{R}$ are given by

$$
\begin{aligned}
\mathcal{R}_I &= -f^{-1}\, e^{ipd/2\hbar} \\
\mathcal{R}_R &= f^{-1}\, R(p'_R) e^{ip'_R d/\hbar}\, e^{ipd/2\hbar} \\
\mathcal{R}_{Rj} &= \frac{R(p'_j) e^{ip'_j d/\hbar}\, e^{ipd/2\hbar} F_j}{\left(p+p'_j+i\hbar 0^+\right) f} \\
\mathcal{R}_{Cj} &= \frac{-2iC(p'_j) e^{ip'_j d/2\hbar} \sin[(p-p''_j)d/2\hbar] F_j}{\left(p-p''_j\right) f} \\
\mathcal{R}_{Dj} &= \frac{-2iD(p'_j) e^{ip'_j d/2\hbar} \sin[(p+p''_j)d/2\hbar] F_j}{\left(p+p''_j\right) f} \\
\mathcal{R}_T &= f^{-1}\, T(p'_T) e^{ip'_T d/\hbar}\, e^{-ipd/2\hbar} \\
\mathcal{R}_{Tj} &= -\frac{T(p'_j) e^{ip'_j d/\hbar} e^{-ipd/2\hbar} F_j}{\left(p-p'_j-i\hbar 0^+\right) f},
\end{aligned}
\tag{18}
$$

where

$$
F_j \equiv \frac{\Omega(p')}{d\Omega(p')/dp'}\Big|_{p'=p'_j}. \tag{19}
$$

Taking into account the integral expression of the $w$-function, $w(z) = e^{-z^2}\, erfc(-iz)$ [34],

$$
w(z) = \frac{1}{i\pi} \int_{\Gamma_-} \frac{e^{-u^2}}{u-z}\, du, \tag{20}
$$

where $\Gamma_-$ goes from $-\infty$ to $\infty$ passing below the pole, and the relation $w(-z) = 2e^{-z^2} - w(z)$, the wave function may finally be written as

$$
\begin{aligned}
\psi(p,t) = if\tau\hbar h^{-1/2}\, e^{-\left(\delta_x p_c^2/\hbar^2\right)+\eta^2} \Big\{ & i\pi\mathcal{R}_I w(u_I) - i\pi\mathcal{R}_R w(-u_R) \\
& - i\pi\mathcal{R}_T w(-u_T) - i\pi \sum_{j=1}^{\infty} [\mathcal{R}_{Rj}+\mathcal{R}_{Cj}+\mathcal{R}_{Dj}+\mathcal{R}_{Tj}] w(-u_j)
\end{aligned}
$$

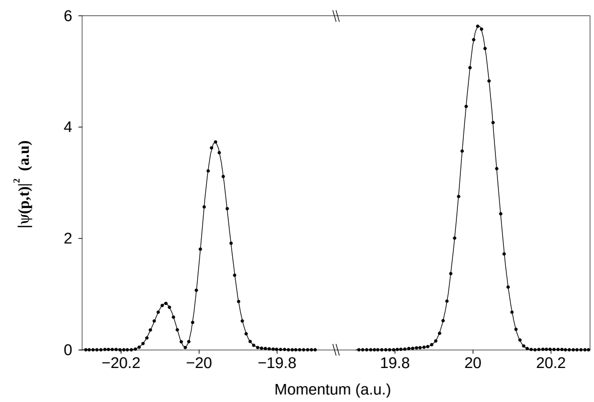


**Figure 1.** $|\psi(p,t)|^2$ as a function of momentum at $t=5$ a.u., when the collision has been completed. The solid line corresponds to the exact solution, whereas the dots correspond to the reflection and transmission (structural) terms and three resonance pole terms from (21). Atomic units are used in all the calculations, and $m=1$. $p_c=20$, $d=2.5$, $V_0=188$, $\delta_x=100$ and $x_c$ is located 50 atomic units to the left of the center of the barrier potential.

$$+\int_{-\infty}^{\infty}[h_R(u)+h_C(u)+h_D(u)+h_T(u)]e^{-u^2}du\Big\}, \tag{21}$$

which is the main result of this paper. The remaining Gaussian integrals are quite generally only a minor correction and may be evaluated with a few terms of the series

$$h(u)=\sum_{n=0}^{\infty}h^{(n)}(0)\frac{u^n}{n!}, \tag{22}$$

which gives

$$\int_{-\infty}^{\infty}h(u)e^{-u^2}du=\sqrt{\pi}\left[h(u=0)+\sum_{n=1}^{\infty}\frac{1\times 3\times ...\times(2n-1)}{2^n(2n)!}h^{(2n)}(u=0)\right]. \tag{23}$$

Note the form of the solution in (21). There are structural terms associated with incidence, transmission and reflection ($I$, $T$, and $R$ terms for short), resonance terms, and the $h$-corrections of (23).

## 3. Examples

In many cases just a few terms in (21) provide an accurate approximation to the exact result. If only the asymptotic behaviour, after the collision has been completed, is of interest, the structural terms $R$ and $T$, associated with reflection and transmission, plus a few resonance pole contributions (again for reflection and transmission) are quite sufficient. The number of resonance poles that have to be added depends on the energy of the collision. In figure 1, for example, we show a case where only three resonance poles have been used in the $R$ and $T$ terms, and no correction term from Eq. (23) has been included.

There are also cases where only two terms are required *during* the collision: the collision with a very opaque barrier ($R$ and $I$ terms), see Fig. 2, and collisions for

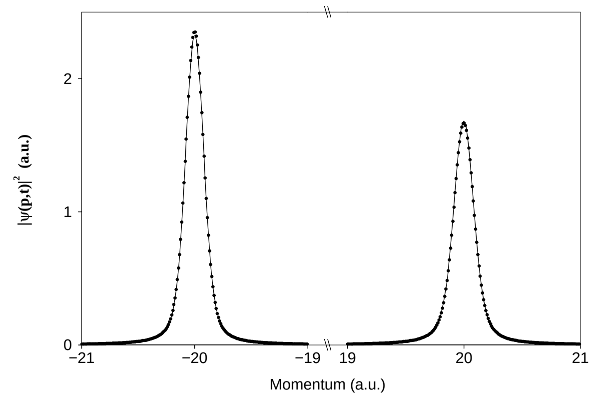


**Figure 2.** $|\psi(p,t)|^2$ as a function of momentum, at $t = 2.5$ a.u., during the collision process. The solid line corresponds to the exact solution whereas the dots correspond to incidence and reflection structural terms of (21) only, and no resonance poles taken into account. $p_c = 20$, $d = 3$, $V_0 = 400$, $\delta_x = 100$, and the initial wave packet is centered 50 atomic units to the left of the barrier center.

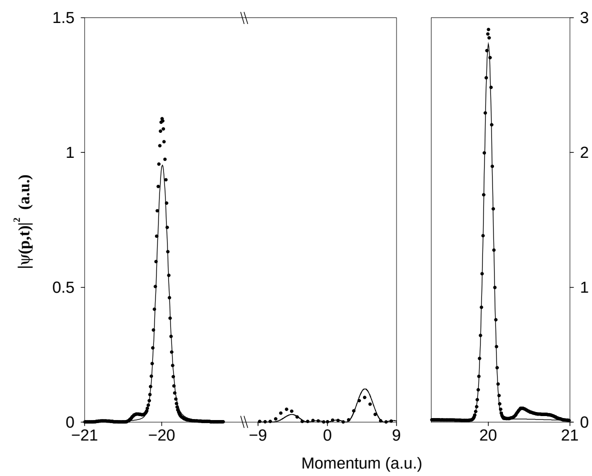


**Figure 3.** $|\psi(p,t)|^2$ as a function of momentum, at $t = 2.7$ a.u., during the collision process. The solid line corresponds to the exact solution, whereas the dots correspond to taking from (21) incidence, reflection, transmission, and barrier ($C$ and $D$) terms, plus three resonance pole terms. When one correction term (23) is added, the approximate result is indistinguishable from the exact one. Same barrier and wave packet parameters as in Fig. 1

very broad an energetic wave packets ($I$ and $T$ terms). This later case has been used recently to explain a transient, classically forbidden enhancement of the high momentum components [35, 36] as an incidence-transmission interference effect [11].

In Figure 3, the case of a very general (typical) situation is depicted. Incidence, reflection, transmission, and barrier ($C$ and $D$) terms from (21), plus three resonance pole terms provide a fairly good approximation for the wave function at an intermediate time during the collision, although the approximate solution clearly overestimates the exact value at the reflection and transmission peaks, and for values of momentum between 20.3 and 21 a.u.. The inclusion of the first correction term in (23) leads to a curve which is indistinguishable in the scale of the figure from the exact result.

Let us also note that (21) is suitable for asymptotic analysis (e.g. short and large times) by means of the asymptotic series of the $w$-function, see e.g. [28, 27]. The $w$-functions may be considered the elementary propagators of the Schrödinger transient modes [37] and play a prominent role in the explicit solution given in (21).

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## Appendix A. Calculation of the resonance poles

The resonance poles are obtained by solving the transcendental equation $\Omega(p') = 0$. A systematic way to do it is based on the differential equation [38]

$$\frac{dp'}{dV_0} = \frac{idV_0\sqrt{m} - p'}{V_0\left(\frac{idp'}{\sqrt{m}} - 2\right)}. \tag{A.1}$$

As boundary condition for the integration of (A.1) we take $p' = 0$ at

$$V_0 = -\frac{n^2\pi^2}{2d^2}; \qquad n = 0, \pm 1, \pm 2, ... \tag{A.2}$$

The integration of (A.1) has to be carried out until the value of $V_0$ corresponds to the physical barrier we want to examine. The integration however cannot be performed along the real axis because of the factor $V_0$ in the denominator of (A.1). To avoid the singularity at $V_0 = 0$, an imaginary term is added to the potential, analytically continuing the differential equation. A parabolic path has been used across the complex $V_0$ plane from the initial values of $V_0$ in (A.2) to the final real value of $V_0$.

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